| | | |
|---|---|---|
| ESRF | **Experiment title:**<br>XAFS measurement of $(Fe,Mn)_2(P,Si)$ compounds at various temperatures | **Experiment number**:<br>26-01-966 |
| **Beamline**:<br>BM26A | **Date of experiment**:<br>from: 28 jun 2013 to: 02 jul 2013 | **Date of report**:<br>05 January 2015 |
| **Shifts:**<br>12 | **Local contact(s)**:<br>D. Banerjee | *Received at ESRF:* |


**Names and affiliations of applicants** (* indicates experimentalists):

Maurits BOEIJE *, TU Delft, Applied Sciences, TU Delft, The Netherlands

Yibole YIBOLE *, TU Delft, Applied Sciences, TU Delft, The Netherlands

Francois GUILLOU *, TU Delft, Applied Sciences, TU Delft, The Netherlands

Niels VAN DIJK*, TU Delft, Applied Sciences, TU Delft, The Netherlands

Ekkes BRÜCK, TU Delft, Applied Sciences, TU Delft, The Netherlands

Dipanjan BANERJEE *, ESRF, Grenoble, France


**Report:**

$(Fe,Mn)_2(P,Si)$ compounds show a ferromagnetic to paramagnetic first-order phase transition at their Curie point, which is around room temperature. Calculations show a redistribution of the electron density around Fe when the transition is crossed, which is not the case for Mn[1].

The aim of this experiment was to monitor the change in the absorption spectra below and above the transition temperature. X-ray Absorption Fine Structure experiments were performed at beamline BM26A. By using a monochromatic beam with an a energy of energy of 7.1 keV, the absorption of the Fe K-edge can be studied. A beam with an energy of 6.5 keV was used to verify that no changes take place at the Mn K-edge.

The redistribution in electron density could lead to a valence change, which would be detected by comparing the XANES part of the spectrum below and above the transition. No significant changes were found for both the Fe or Mn spectra. The EXAFS spectra indicate the local electronic environment and these change across the transition. The Fourier transform of the reduced data showes an additional peak, which was not expected based on the crystallographic data (fig 1). This peak was found to shift as the material crosses the transition temperature, which is around 280 K (fig 2).

When fitting the data, the best fits were obtained by including electron density at the *2e* and *6j* sites. The actual electron charge which is responsible for these peaks was found to be constant and of the order of 0.3 electrons. The spectra for Mn remain unchanged across the transition.

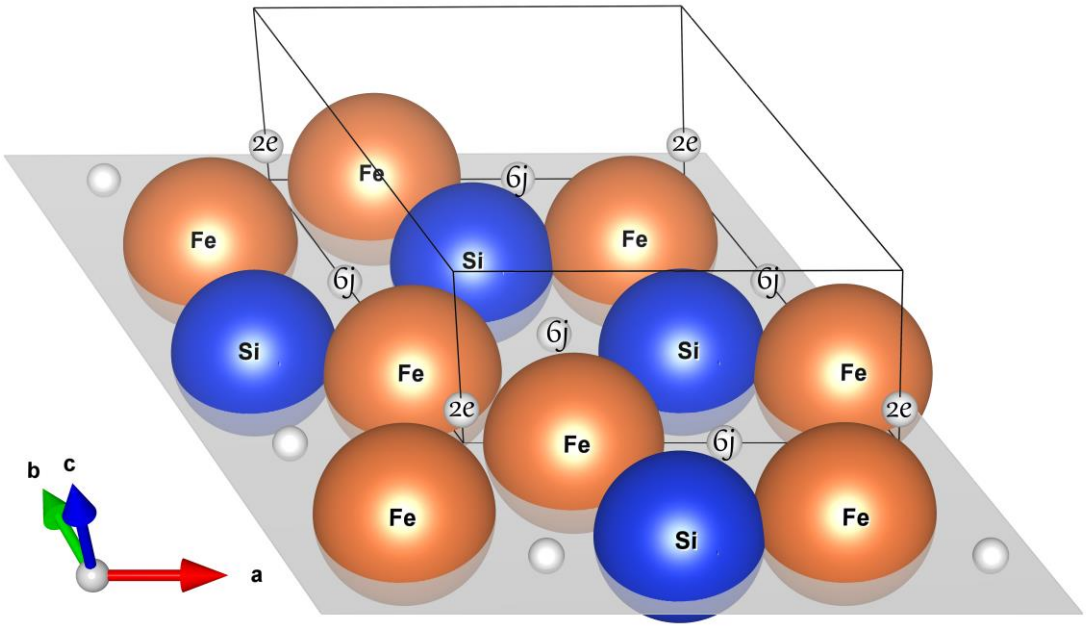


*Fig. 1: Slice of Fe layer of the unit cell of $(Fe,Mn)_2(P,Si)$ compounds. The Mn layer is above the Fe layer and is not shown. The Fe and Mn atoms occupy the 3f and 3g Wyckoff positions respectively. The Si and P atoms occupy both the 1b and 2c positions.*

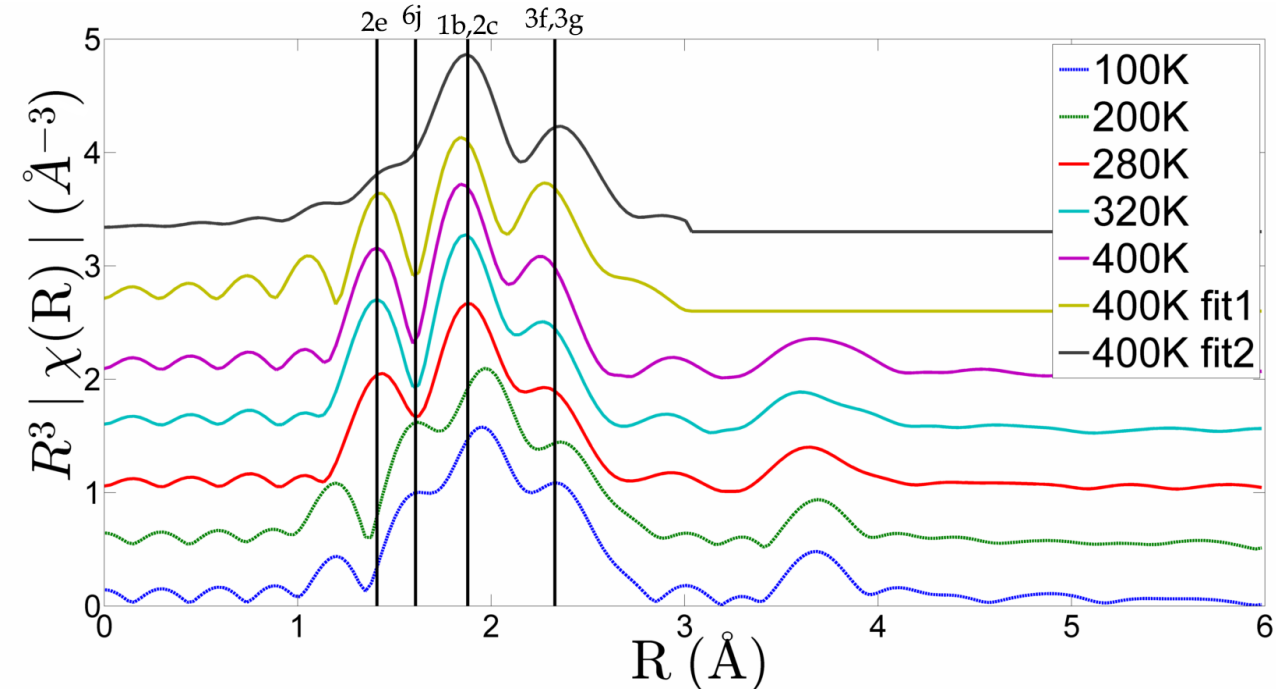


*Fig. 2: Fourier transform of the reduced data obtained by measuring the absorption spectrum of the Fe k-edge. The peak at the third line is due to the scattering of the photoelectron with the P,Si atoms. The peak at the fourth line is due to the scattering on the Fe,Mn atoms. An additional peak was found at shorter distances, corresponding to the 2e and 6j positions. Two fits of the data are presented, one only considering atomic contributions and one including electron density at the 2e site.*

**Reference:**

[1] N. Dung, Z. Ou, L. Caron, L. Zhang, D. Thanh, G. de Wijs, R. de Groot, K. Buschow, and E. Brück, Advanced Energy Materials 1 (2011) 1215–1219.